

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.78e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.84e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl cinnamate</div> <div>Measured: 1.00e-05</div> <div>Predicted: 1.73e-02</div>	<div>Image not found</div> <div>Butam</div> <div>Measured: 1.19e-06</div> <div>Predicted: 8.05e-04</div>	<div>Image not found</div> <div>Carbonic acid, di-2-propen-1-yl ester</div> <div>Measured: 1.72e-07</div> <div>Predicted: 2.67e-01</div>
<div>Image not found</div> <div>Nonylphenyl diphenyl phosphate, mixed isomers</div> <div>Measured: 1.72e-04</div> <div>Predicted: 8.08e-09</div>	<div>Image not found</div> <div>Heptenophos</div> <div>Measured: 1.72e-04</div> <div>Predicted: 3.05e-04</div>	